S-matrix network models for coherent waves in random media: construction and renormalization

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Abstract. Networks of random quantum scatterers (S-matrices) form paradigmatic models for the propagation of coherent waves in random media. S-matrix network models cover universal localization-delocalization properties and have some advantages over more traditional Hamiltonian models. In particular, a straightforward implementation of real space renormalization techniques is possible. Starting from a finite elementary cell of the S-matrix network, hierarchical network models can be constructed by recursion. The localization-delocalization properties are contained in the flow of the forward scattering strength ('conductance') under increasing system size. With the aid of 'small scale' numerics qualitative aspects of the localization-delocalization properties of S-matrix network models can be worked out.

Keywords: S-matrix network models, Localization-delocalization transition, renormalization group, multifractality

1 Introduction

Localization and fluctuation phenomena are fascinating universal features in any disordered coherent wave mechanical system. In 1982 Shapiro [1] pointed out that a convenient modeling of disordered coherent wave mechanical systems can be given by networks of unitary random scattering matrices. This modeling covers essential symmetries and characteristic length scales, but does not rely on particular dispersion relations and specific details. Therefore, it is of relevance in various fields of theoretical physics, e.g. in optics, mesoscopic electronics, and quantum chaos. Smatrix network models (NWMs) have a number of advantages over more traditional Hamiltonian models. NWMs yield directly transport quantities [2], wave packet dynamics [3], and quasi-energy eigenvalues and eigenstates [4]. A well known NWM introduced by Chalker and Coddington (CC-model) [7] (see also [8]) describes the situation of disordered two-dimensional (2D) electrons undergoing the quantum Hall localization-delocalization (LD) transition in a strong perpendicular magnetic field. A major advantage of S-matrix NWMs is a straight forward implementation of real space renormalization group (RG) techniques [5, 6] which open new perspectives for investigating LD transitions.

Here we address the construction of S-matrix NWMs starting from symmetry considerations and/or from an Anderson tight-binding Hamiltonian. We discuss alternative implementations for a RG action. To reach a qualitative overview of phases in the phase space of scattering strengths one can construct hierarchical network models for which a RG algorithm can be formulated that is designed for 'small scale' numerics. The construction of S-matrix NWMs and the RG methods are demonstrated on particular two-dimensional models.

2 Construction of S-matrix networks

Quite generally, a NWM can be constructed as follows. Take a regular network of $\mathcal N$ sites and N bonds. Each bond α carries propagating wave modes (n_{α}^+) incoming modes and n_{α}^- outgoing modes) represented by complex amplitudes, $\psi_{n_{\alpha}^+}$. On the sites unitary S-matrices map incoming to outgoing amplitudes. The elements of each S-matrix are (in general) random quantities respecting the symmetries of S and are characterized by typical scattering strengths. Random phases are attached to the amplitudes on the bonds. They simulate the random distances between scatterers in realistic systems.

2.1 Topology and site S-matrix

The construction of a NWM is fixed by the choice of a certain type of random S-matrix and a $\mathcal{N} \times \mathcal{N}$ connectivity matrix C which has elements $C_{ij} = 1$ if a wave mode can propagate from site i to site j and $C_{ij} = 0$ otherwise. The NWM defines a dynamical system by S and C. Together they lead to a unitary matrix U [8, 9, 10] called 'network operator'. It maps all incoming to outgoing wave modes. We choose a convenient time unit and denote the vector of the $B \propto N$ bond amplitudes as ψ such that $\psi(t+1) = U\psi(t)$. The eigenphases ϕ_n (n = 1...B) and corresponding eigenvectors ψ_n of U, $U\psi_n = \exp(i\phi_n)\psi_n$, can then be interpreted as quasi-energies and corresponding eigenstates.

2.2 Two-dimensional networks

Let us now report on two-dimensional NWMs with the topology of a square lattice and a connectivity matrix that connects each site with its four nearest neighbors. The corresponding S-matrix is graphically represented in Fig. 1 and reads

$$S = \begin{pmatrix} r^1 & d_R^{21} & t^{31} & d_L^{41} \\ d_L^{12} & r^2 & d_R^{32} & t^{42} \\ t^{13} & d_L^{23} & r^3 & d_R^{43} \\ d_R^{14} & t^{24} & d_L^{34} & r^4 \end{pmatrix} . \tag{1}$$

The parameters of each S-matrix are the amplitudes of transmission t, reflection r, and deflection to the left d_L and right d_R which contain random phases compatible with symmetry requirements. Scattering strengths of a site S-matrix allow to define

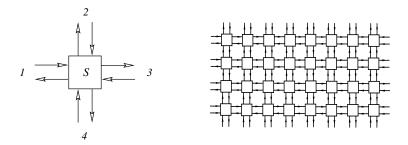


Fig. 1: U2 network model with unitary S-matrices. On the left the elementary S-matrix and on the right a section of the whole network are graphically represented.

transport mean free paths l_e (measured in units of the lattice constant) for a prescribed forward direction by $1/l_e = (1-T)/T$. Here T is the probability to be transmitted in the prescribed forward direction. Such definition is known from the scattering theoretical approach to quasi-1D systems (e.g. [11]).

The unitarity of the S-matrix requires $|t|^2 + |r|^2 + |d_L|^2 + |d_R|^2 = 1$. The corresponding parameter space of scattering probabilities, a quarter of a pyramid, is shown in Fig. 2 and forms the phase space of the U2-model ('U' stands for unitary, '2' for the two-dimensional lattice structure). The points in the corners of the phase space are the

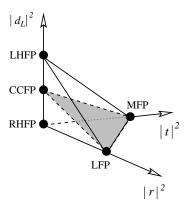


Fig. 2: The three-dimensional phase space of the U2-model is spanned by scattering strengths $0 < |t|^2, |r|^2, |d_L|^2 < 1$ with $|t|^2 + |r|^2 + |d_L|^2 = 1 - |d_R|^2$ and $|d_R|^2 < 1$. The shaded area corresponds to the U2NC-model for which $|d_L| = |d_R|$. The points LHFP, RHFP, LFP and MFP are characterized by $|d_L| = 1$, $|d_R| = 1$, |r| = 1 and |t| = 1, respectively. They form the corners of the U2-phase space. The critical fixed point of the Chalker-Coddington model (CCFP) corresponds to $|d_L|^2 = |d_R|^2 = 1/2$.

metallic fixed point (MFP) (|t| = 1), the localization fixed point (LFP) (|r| = 1), and the left (right) handed fixed point LHFP (RHFP), $|d_L|^2 = 1$ ($|d_R|^2 = 1$). The term 'fixed point' refers to the renormalization group action to be discussed below.

2.3 Symmetries and phase space

In the absence of handedness of the scattering process, i.e. $|d_L| = |d_R|$, the model is denoted as non-chiral (U2NC-model). The phase space of the U2NC-model corresponds to the shaded plane in Fig. 2. The point of $|d_L|^2 = |d_R|^2 = 1/2$ is denoted as Chalker-Coddington fixed point (CCFP) since the U2-model reduces to two uncoupled CC-models for vanishing t and r and the phase space of the CC-model is one-dimensional (1D) and parameterized by the values of $T := |d_L|^2$ (see Fig. 3a). Further symmetries of the S-matrix lead to a reduction of the number of independent parameters. This typically eliminates random phases, but can also lead to restrictions in the phase space of scattering strengths. For time reversal symmetric scattering in the U2NC-model the S-matrix is symmetric and the phase space is reduced by $|r| + |t| \ge 1$. The model is then denoted as O2NC-model where 'O' stands for orthogonal (the network operator can be diagonalized by orthogonal matrices). Its phase space is shown in Fig. 3b. Imposing symmetry constraints reflecting a sublattice structure, e.g. $\Sigma_3 S \Sigma_3 = S^{\dagger}$, where $\Sigma_3 := \text{diag}(1, 1, -1, -1)$, the U2NC-model becomes ' Σ_3 -

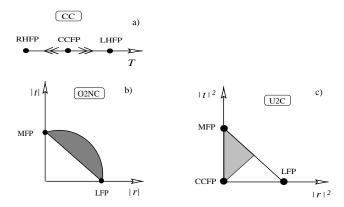


Fig. 3: a) The phase space of the Chalker-Coddington model. Two of the fixed points correspond to quantum Hall plateaus (LHFP and RHFP), the critical point CCFP corresponds to the plateau to plateau transition. b) The phase space of the O2NC-model in |r|, |t| parameter space. The time reversal symmetry leads to the restriction $|t| + |r| \ge 1$ (grey area). c) The phase space of a chiral model. The chiral symmetry (see text) leads to the restriction $|t|^2 \ge |r|^2$ (grey area).

chiral'. Although $|d_L| = |d_R|$ is still valid, the chiral symmetry leads to further phase space constraints, e.g. to $|r|^2 \le |t|^2$ (for $d \ne 0$) for Σ_3 -chirality (Fig. 3c).

2.4 From tight binding models to S-matrix networks

So far S-matrix network models appeared as models on their own, dictated by topology and symmetry. However they can also appear as the result of a mapping from a microscopic Hamiltonian, as is the case for the CC-model [8]. In this subsection we show how tight binding models can also lead to S-matrix network models. This opens a new flexibility in the methods to study these models.

The general idea is to take a typical microscopic cell of a given tight binding model and attach 1D semi-infinite leads to it, as many as is appropriate for topology and symmetry aspects. Then calculate the S-matrix of this device. It may then serve to define a NWM.

We proceed as follows. The Hamiltonian $H=H_0+H_1$ is decomposed into a part that describes only the leads, H_0 , and the part that describes the microscopic cell together with its coupling to the leads, H_1 . The scattering states with continuous spectrum are chosen to obey energy normalization $\langle \alpha(E)|\alpha(E')\rangle = \delta(E-E')$. Then the S-matrix is given as $S_{\alpha\beta} = \delta_{\alpha\beta} - 4\pi i T_{\alpha\beta}$ where the T-matrix (operator) is related to the resolvent (Green's function) $G^+ = (E+i0^+-H)^{-1}$ by $T=H_1+H_1G^+H_1$. Note that H_0 describes 'isolated' terminals, i.e. (semi-infinite leads) and the modes $|\alpha\rangle$ contain both 'in'- and 'out'-states. Introducing the projector Q=1-P onto the Hilbert-space of the terminal states the T-matrix elements read

$$T_{\alpha\beta} = \left\langle \beta \mid H_{QP}G_{PP}^{+}H_{PQ} \mid \alpha \right\rangle. \tag{2}$$

The projected Green's function G_{PP}^+ can be determined by a non-hermitian effective Hamiltonian defined entirely on the P-space, i.e. we have to invert a V dimensional matrix when V is the number of sites in the microscopic cell.

It is convenient to treat the terminals as semi-infinite 1D tight-binding models with only kinetic energy and unit hopping strength. The terminal Green's function as well as the amplitudes of the terminal states can be calculated analytically. Together with the solution of the $V \times V$ matrix problem the S-matrix can be obtained from Eq. (2). To make the discussion more explicit we present the results for two models [12]. First consider the microscopic cell in Fig. 4a consisting of a on-site random energy ε attached to four terminals. For energies in the band center of the 1D terminals the scattering matrix elements are [13]

$$t = d_L = d_R = \frac{8 - 2i\varepsilon}{16 + \varepsilon^2}$$

and r = 1 - t. The model is a member of the O2NC-model since S is symmetric. To get scattering strengths characteristic for an ensemble of disorder realizations one should average them with respect to an appropriate distribution of ε .

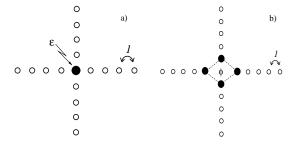


Fig. 4: Elementary S-matrix for tight binding Hamiltonian models: a) A central site with random on site energy ε is coupled to four semi-infinite leads (terminals) characterized by unit hopping amplitudes. b) Four central sites enclosing a random flux ϕ are coupled to semi-infinite leads.

Second we address a microscopic cell for the random flux problem as shown in Fig. 4b. No on-site disorder is introduced, but a random flux phase ϕ (the flux quantum is set to 2π) is picked up when moving around the four inner sites (anti-clockwise). At the band center the resulting scattering amplitudes (for an incoming wave from the left in Fig. 4b) are found to be

$$\begin{array}{rcl} r & = & (4\sin^2(\phi/2)-1)/D\,,\; t=-4\cos(\phi/2)/D\,,\\ d_L^{12}(\phi) & = & e^{-i\phi/4}(2ie^{i\phi}-4i)/D=-(d_R^{21})^* \end{array}$$

with $D=4\sin^2(\phi/2)+5$. A close inspection shows that the model is ' σ_3 -chiral', i.e. $\sigma_3 S \sigma_3 = S^{\dagger}$ with $\sigma_3 := \text{diag}(1,-1,1,-1)$. This property is lost for energies not exactly at the band center.

3 Implementation of a renormalization group

To detect localized, critical and delocalized phases of an infinite NWM one likes to implement a convenient renormalization group (RG). Following the scaling theory of Abrahams et al. [14] one could think of computing the two-probe conductance g(L) for a network of size L^2 (Fig. 5a). This involves strong mesoscopic fluctuations in g(L). For that reason the self-averaging object $\Lambda(M) = \xi(M)/M$ has been introduced [15]

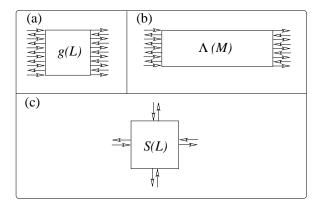


Fig. 5: Different ways of implementing a renormalization group: a) The two probe conductance g(L) is studied for increasing system size L. b) The finite size scaling variable $\Lambda(M)$ is studied as a function of width M in quasi-1D geometries. c) The elementary S-matrix can be generalized to an S-matrix S(L) for arbitrary system size L.

to study the scaling behavior. Here $\xi(M)$ is the localization length corresponding to quasi-1D geometries (Fig. 5b) of length $L \to \infty$ and finite width M. This so called 'finite size scaling' method is the 'first choice' method for numerical investigations of scaling properties [16]. It has been successfully applied to the CC-model [7, 17] and to the U2NC-model (and variants of it) [18]. Still, it involves 'large scale' numerics, i.e. powerful computation units and/or large storage capacities. One reason for this is that the finite size scaling is an 'exact' numerical method – no approximations in the modeling are involved.

Alternatively, one can treat the whole system of linear size L^2 as a big scattering unit (see Fig. 5c) giving rise to a RG flow of the S-matrix: $S_{\alpha\beta}(1) \longrightarrow S_{\alpha\beta}(L)$. Consequently, this RG procedure allows to study a RG flow in the phase space of scattering strengths. In particular the fixed points of this RG flow are of interest. The repulsive or attractive behavior of the RG flow close to the fixed points gives valuable information about phase transitions. For example, the CCFP is repulsive within the phase space of the CC-model while LHFP and RHFP are attractive fixed points (see Fig 3a). These simple facts contain essentials of the quantum Hall effect.

4 Hierarchical S-matrix networks

The numerical effort in computing a single S-matrix element of S(L) is of the same order as in computing a single eigenstate of the network operator U. Furthermore, one needs computations for different disorder realizations to take large fluctuations into account. Thus, a further idea is needed to make advantage of the RG flow in phase space. We give up the 'exactness' of the RG method and consider simplified NWMs by recursive constructions of 'hierarchical' NWMs as shown in Fig. 6 for the U2-model. A section of a given NWM containing b^2 sites and V 'active' elementary S-matrices (S-matrices with only trivial elements 0,1 are not counted as active) is taken. The scatterers are connected such that the resulting network has the same terminal structure as each of the elementary S-matrices. Accordingly, the hierarchical models are denoted as [b/V]-models. The hierarchical models have fractal dimension

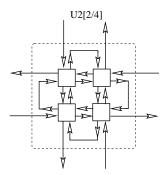


Fig. 6: An example (denoted as U2[2/4]) for a recursive construction of a hierarchical network model. Four elementary S-matrices are connected such that the resulting 4×4 network has the same terminal structure as each of the elementary S-matrices.

 $D^{[b/V]} = \ln V/\ln b$. In the $V \to \infty$ limit the original NWM may be recovered exactly (depending on the construction). Obviously, the RG flow works by recursion and the computational effort simplifies drastically. The hierarchical NWMs approximate the original ones in an uncontrolled manner. Better approximations can only be gained by increasing the size of the elementary cell and by studying the convergence of quantitative results, e.g. critical exponents. However, qualitatively correct results for the existence or non-existence of phase transitions can be obtained already for moderate sizes of the elementary cells. The RG method for hierarchical NWMs yields qualitative aspects of the RG flow in phase space of the original NWM relying on small scale numerics.

5 Renormalization algorithm

In the following we outline the six-step algorithm of the RG in hierarchical network models.

- (i) In the first step $S_{\alpha\beta}(L=b)$ is determined as a function of the scattering matrix elements of all active scatterers for a given elementary cell (respecting unitarity constraints). For small numbers V this can be done by hand or computer algebra.
- (ii) The set of scattering strengths **T** is drawn from an initial distribution, $P_0(\mathbf{T})$. Phases are taken uncorrelated and uniformly distributed in the interval $[0, 2\pi]$. For each realization $\mathbf{T}(L=b)$ is calculated with the help of the algebraic expression obtained in the first step.
- (iii) After collecting a large number ($\sim 10^3$) of scattering strengths an approximate distribution function $P_{L=b}(\mathbf{T})$ is determined which depends on the initial distribution $P_0(\mathbf{T})$. In particular, it yields the average value $\langle \mathbf{T} \rangle$ (L=b) and other characteristic parameters of the distribution.
- (iv) Steps (ii) and (iii) are repeated, but now **T** is drawn from the distribution $P_{L=b}(\mathbf{T})$ obtained before. This leads to a reasonable approximation for $P_{L=b^2}(\mathbf{T})$ and for $\langle \mathbf{T} \rangle$ ($L=b^2$).
- (v) Step (iv) is repeated N times $(N \sim 10^1)$ which yields, for each initial distribution $P_0(\mathbf{T})$, the flow of the distribution function $P_L(\mathbf{T})$ and of the mean $\langle \mathbf{T} \rangle (L)$ as functions of $\ln L = (N+2) \ln b$.

(vi) Finally, the RG process ((i) – (v)) will be repeated for a number of different initial distributions $P_0(\mathbf{T})$ to study the RG flow of typical values close to the fixed points.

6 Small scale numerics

RG calculations following this algorithm have been performed for the CC-model [6] (see also [5]) and the Manhattan model (MM) considered in [19]. The MM is defined by r=0 and an alternating structure of $d_L=0$ or $d_R=0$ (see Fig. 8) leaving the forward transmission $T:=|t|^2$ as the single parameter for its phase space.

The results for a number of CC[b/V]-models [6] can be summarized as follows: A LD transition occurs, characterized by a repulsive fixed point distribution $P^*(T)$ (here $T := |d_L|^2$) which is broad over the interval [0,1]. After a few iteration steps the flow becomes independent of the initial distribution and can be characterized by the average value $\langle T \rangle$. The critical distributions were found to be symmetric around the critical mean value $T^* = 0.5$ and developed a shallow minimum there. The critical distribution for the CC[3/5]-model and the scaling of its mean value is shown in Fig. 7. Furthermore, one observes that with increasing elementary cells the critical exponent of the localization length approaches the value of the original CC-network in a monotonic way from above.

In addition to the localization length exponent a second critical exponent is required to characterize the LD transition, the critical exponent, $\alpha_0 - D$, of the order parameter (the typical density of states) [20]. This quantity scales to zero at the critical point,

$$\rho_{\rm t}(L) \propto L^{-(\alpha_0 - D)} , \ \alpha_0 > D ,$$

since critical states are not totally space-filling, but multifractal. Here D is the dimension of the system which may be fractal in hierarchical NWMs. Adopting the method of Klesse and Metzler [9] to calculate wave functions as eigenstates of the network operator U the multifractal exponent α_0 can be computed for a given network model. To reduce the computational effort, all scattering strengths can be fixed to the critical value T^* . Moderate sizes ($L \approx 50$) are used and several realizations to obtain α_0 . It turns out that $\alpha_0 - D^{[b/V]}$ monotonically approaches the value of the CC-model [9] from above as $D^{[b/V]}$ approaches d=2 from below.

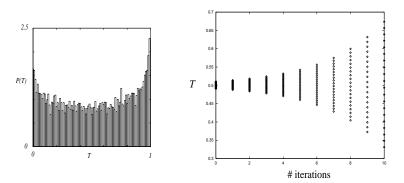


Fig. 7: The critical distribution of scattering strengths (left) and the corresponding flow of average transmission strengths T under increasing number of renormalization steps (right) for the CC[3/5]-model.

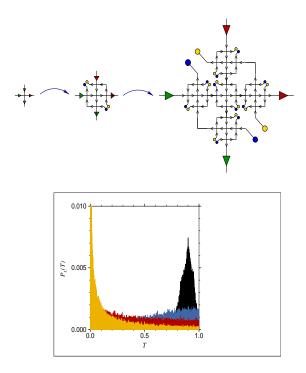


Fig. 8: The [3/5]- model corresponding to the Manhattan model (top) and the flow of the distribution of the forward scattering strength (bottom) under renormalization (L = 3, 9, 27, 81) to strong localization. Amplitudes on open ends with the same symbol (bullet or shaded circle) are identified within one RG step.

It is believed that a crucial ingredient of the CC-model is its handedness reminiscent of the strong magnetic field in quantum Hall systems. To check whether the handedness is essential for the occurrence of the LD transition we performed a RG process for the Manhattan model which has a one-dimensional phase space like the CC-model, but no handedness (even for strong deflection there are as many right circulating loops as left circulating loops in a large network). Indeed, we find no indication for a LD transition in the MM. Instead, any initial distribution of the forward scattering strength T flows to the strong localization fixed point LFP (see Fig. 8).

7 Conclusions

S-matrix network models provide a flexible tool to study disordered coherent wave mechanical systems. The construction can be based on topology and symmetry requirements, but also on microscopic models such as tight binding Hamiltonians. For a given network model a recursive construction of associated hierarchical network models can be performed. Iterating this construction yields an approximation of the original network model which allows to study the flow of scattering strengths in the phase space of the network model by a six step renormalization group algorithm. The precision of critical parameters obtained by this procedure can be improved by increasing the number of realizations in each iteration step. The critical parameters are then more precise for the particular hierarchical model, however have uncontrolled

deviations from that of the original model. Better approximations can only be gained by increasing the size of the elementary cell and studying the convergence of critical exponents. The computational effort then drastically increases and becomes comparable to that of the well known finite size scaling method based on the transfer matrix technique. The advantage of the RG method for hierarchical network models is that it yields qualitative aspects of the RG flow in phase space of the original model using only small scale numerics.

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References

- [1] B. Shapiro, Phys. Rev. Lett. 48,823 (1982).
- [2] M. Metzler, PhD thesis, Universität zu Köln, unpublished (1997); M. Janssen, M. Metzler, M.R. Zirnbauer, unpublished.
- [3] B. Huckestein, R. Klesse, Phil. Mag. B 77, 1181 (1998)
- [4] R. Klesse, M. Metzler, Phys. Rev. Lett. 79, 721 (1997).
- [5] A.G. Galstyan, M.E. Raikh, Phys. Rev. B 56, 1422 (1997); D.P. Arovas, M. Janssen,
 B. Shapiro, Phys. Rev. B 56, 4751 (1997).
- [6] A. Weymer, M. Janssen, Annalen der Physik 7, 159 (1998).
- [7] J.T. Chalker, P.D. Coddington, J. Phys.C 21, 2665 (1988).
- [8] H.A. Fertig, Phys. Rev. B 38, 996 (1988).
- [9] R. Klesse, M. Metzler, Europhys. Lett. 32, 229 (1995).
- [10] I. Edrei, M. Kaveh, B. Shapiro, Phys. Rev. Lett. 62, 2120 (1989); M. R. Zirnbauer, Annalen der Physik 3, 513 (1994); T. Kottos, U. Smilansky, Phys. Rev. Lett. 79, 4794 (1997).
- [11] A.M.S. Macedo, J.T. Chalker, Phys. Rev. B 46, 14985 (1992).
- [12] M. Janssen, unpublished.
- [13] For a two lead configuration the procedure defines a mean free path which is consistent with the one resulting from independent calculations of 1D localization lengths $\xi = 2l_e$ carried out for weak disorder (cf.[16]).
- [14] E. Abrahams, P.W. Anderson, D.C. Liciardello, T.V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
- [15] A. MacKinnon, B. Kramer, Phys. Rev. Lett. 47, 1546 (1981); J-L. Pichard, G. Sarma, J. Phys. C 14, L127 (1981).
- [16] B. Kramer, A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
- [17] D.-H. Lee, Z. Wang, S. Kivelson, Phys. Rev. Lett. **70**, 4130 (1992).
- [18] R. Merkt, M. Janssen, B. Huckestein, Phys. Rev. B 58, 4394 (1998); P. Freche, M. Janssen, R. Merkt, unpublished (cond-mat/9808273).
- [19] M.R. Zirnbauer, J. Math. Phys. 38, 2007 (1997).
- [20] M. Janssen, Phys. Rep. 295, 1 (1998).